Simulating the Langevin force by simple noise in nuclear one-body dynamics

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For the purpose of addressing catastrophic phenomena in nuclear dynamics, we explore the possibility of simulating the stochastic part of the collision integral in the Boltzmann-Langevin model by the numerical noise associated with the finite number of test particles in the ordinary Boltzmann-Uehling-Uhlenbeck (BUU) treatment. Considering idealized two-dimensional matter, for which it is practical to simulate the Boltzmann-Langevin equation directly, we demonstrate that the number of test particles per nucleon can be adjusted so that the corresponding BUU calculation yields a good reproduction of the spontaneous clusterization occurring inside the spinodal region. This approximate method may therefore provide a relatively easy way to introduce meaningful fluctuations in simulations of unstable nuclear dynamics.

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I. INTRODUCTION

Intense experimental and theoretical efforts are currently being directed at understanding the mechanisms responsible for the observed production of complex fragments in heavy-ion collisions. In recent years, intermediate-energy heavy-ion collisions have been studied extensively with Boltzmann-Uehling-Uhlenbeck-(BUU) type models, in which the collisionless Vlasov equation for the reduced one-body phase-space density $f(\mathbf{r},\mathbf{p})$ is augmented by a Pauli-blocked Boltzmann collision term of the Uehling-Uhlenbeck form [1]. The resulting BUU equation describes the average one-body density and is suited for the description of one-body observables, such as inclusive particle spectra. Models of this class have been quite successful in describing the structure of the equilibrated primary sources formed during the first stage of strongly damped and (incomplete) fusion reactions [2].

However, this mean-trajectory approach cannot provide a description of phenomena exhibiting large fluctuations or instabilities, such as multifragmentation processes. In such cases, a fully dynamical picture is essential for predicting particular space geometries in fragment production which should be ultimately related to fundamental properties of nuclear interactions in the nuclear medium. Thus there is a clear need for extending the usual mean-trajectory transport models so as to include fluctuations.

Generally speaking, in order to describe the formation of many fragments one should have to solve the full many-body problem, which is impractical. However, alternative avenues considering ensembles of one-body densities have been investigated [3–8]. These approaches are equivalent to the so-called Boltzmann-Langevin (BL) model in which the stochastic part of the two-body interaction is added to the mean BUU evolution. In particular, using an exact lattice simulation of the BL equation, it was shown [9] that in presence of instabilities, the fluctuations coming from the stochastic part of the collision integral are propagated and amplified by the mean field, leading finally to the formation of clusters. Up to now this approach has been applied only to an idealized two-dimensional system [9], and it appears to be unfeasible to treat a three-dimensional scenario, such as a nuclear collision, because of the large amount of computational effort required.

We have therefore investigated the possibility of replacing the (usually complicated) physical fluctuations by a simpler noise. The main idea is that the dynamics of very unstable systems may be less sensitive to the particular nature of the fluctuations, because the most unstable modes will quickly dominate. Specifically, we study the possibility of replacing the physical fluctuations arising from the collision integral by the numerical noise present when the ordinary BUU model is solved by the test-particle method, as is most commonly done. From a practical point of view, such a simplified approach would allow us to perform approximative calculations for realistic three-dimensional processes.

II. BOLTZMANN-LANGEVIN MODEL

The Boltzmann-Langevin equation can be written in compact form as

$$\dot{f} \equiv \frac{\partial f}{\partial t} + \{f, H[f]\} = I[f] = \bar{I}[f] + \delta I[f] \ , \qquad (1)$$

where $f(\mathbf{r},\mathbf{p},t)$ is the one-body phase-space density. On

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the left-hand side, $H[f](\mathbf{r},\mathbf{p})$ is the self-consistent effective single-particle Hamiltonian governing the collisionless Vlasov evolution. On the right-hand side, $I[f]$ denotes the effect of the residual two-body collisions, which can be decomposed into an average effect $\bar{I}[f]$, and the fluctuating part $\delta I[f]$. The standard BUU treatment retains only the average term $\bar{I}[f]$ and therefore produces a single dynamical trajectory for $f(\mathbf{r},\mathbf{p})$. The fluctuating collision term $\delta I[f]$ acts like a random "kick"on the one-body density and may therefore produce branchings of the dynamics, resulting in a bundle of different histories.

The physical origin of the fluctuations can be understood as follows [8]: The actual number $\mathcal{N}$ of elementary collisions has a Poisson distribution characterized by its mean value $\bar{N}$ and so has the variance $\sigma_N^2 = \bar{N}$. The average part of the collision integral, $\bar{I}[f]$, expresses the evolution corresponding to putting $N = \bar{N}$ for all such elementary processes, while the fluctuating part accounts for the stochastic remainder $\delta N = N - \bar{N}$.

In order to gain insight into the growth of fluctuations, we start from linear response theory, which is valid for small fluctuations and therefore is well suited for describing the early evolution of the system. Let us denote by ν a particular unstable mode of the BUU dynamics, and let its associated imaginary energy be $E_\nu = i\hbar/t_\nu$. Looking at the linear response to the Boltzmann-Langevin evolution, it is possible to demonstrate [10] that early on the average density fluctuation σ_ν^2 in the unstable mode ν satisfies an equation of motion of the form

$$\frac{d}{dt}\sigma_\nu^2 \approx 2D_\nu + \frac{2}{t_\nu}\sigma_\nu \ , \tag{2}$$

where D_ν is the source term arising from the stochastic nature of the collision integral. It can be expressed as [10]

$$2D_\nu = \int \frac{d\mathbf{r}d\mathbf{p}}{h^2} \int \frac{d\mathbf{r}'d\mathbf{p}'}{h^2}\, F_\nu(\mathbf{r},\mathbf{p})\, F_\nu^*(\mathbf{r}',\mathbf{p}') \times\alpha(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}') \ , \tag{3}$$

where $\alpha(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}') = (\partial/\partial t)\langle\delta f(\mathbf{r},\mathbf{p})\delta f(\mathbf{r}',\mathbf{p}')\rangle_{t=0}$ is the early growth rate of the correlation function and $F_\nu(\mathbf{r},\mathbf{p})$ is the eigenmode associated with the unstable mode.

It follows that the fluctuations of the mode ν exhibit the following behavior in time:

$$\sigma_\nu^2(t) \approx D_\nu t_\nu (e^{2t/t_\nu} - 1) + \sigma_\nu^2(0) e^{2t/t_\nu} \ , \tag{4}$$

where $\sigma_\nu^2(0)$ is the initial fluctuation. This result shows that the terms $D_\nu t_\nu$ and $\sigma_\nu^2(0)$ play similar roles in the evolution. Therefore, it may be possible to replace the physical source term D_ν by a suitable initial noise $\sigma_\nu^2(0)$ determined by the relation

$$\sigma_\nu^2(0) = D_\nu t_\nu \ . \tag{5}$$

This is the idea that we will now test in a simplified scenario.

III. TEST IN AN IDEALIZED SYSTEM

In order to make a first quantitative test of the idea described above, we have considered a gas of fermions situated on a two-dimensional torus with side lengths equal to $L_x = 63$ fm and $L_y = 21$ fm. For the effective one-body field we employ a simplified Skyrme interaction

$$U(x) = A\frac{\bar{\rho}(x)}{\rho_0} + B\left(\frac{\bar{\rho}(x)}{\rho_0}\right)^2 , \tag{6}$$

with $A = -100.3$ MeV and $B = 48$ MeV. Moreover, ρ_0 is the saturation density and $\bar{\rho}(x)$ is the average of the density $\rho(x,y)$ with respect to the transverse direction y and folded in the x direction with a Gaussian of width $a = 0.87$ fm. Since the effective field U then depends on x only, the same holds for those modes that can be excited, and this simplifies the analysis considerably. The folding simulates the finite range of the interaction, which introduces a natural cutoff scale for the unstable modes. In determining the parameters of U, we have sought to mimic standard three-dimensional matter. Thus we have required a Fermi momentum of $P_F = 260$ MeV/c, a binding energy of 16 MeV per nucleon, and that the density doubling lead to approximately zero binding (corresponding to a compressibility modulus of $K \approx 300$ MeV for a calculation in three dimensions). The in-medium "cross section" was taken as 2.4 fm, corresponding to an interaction radius of 1.2 fm. In the present idealized two-dimensional system, the saturation density is $\rho_0 = 0.55$ fm^{-2}. In order to ensure that the system is initially situated inside the spinodal region, we prepare the system to have a uniform density equal to half the normal density, $\rho(x,y,t=0) = \frac{1}{2}\rho_0$, and to have a temperature of $T = 3$ MeV. This physical scenario is similar to what was considered in Ref. [9].

A. Lattice simulation

Recently a lattice simulation of the BL evolution was developed [7–9]. In this method the stochastic part of the collision number, $\delta N(12;1'2')$ (see above), is simulated directly on a lattice in phase space. The size of the phase-space cells must be of the order h^2 in order to simulate the extension of an elementary quantum state, and we have used $\Delta x = 3$ fm and $\Delta p = 120$ MeV/c. The mean-field evolution is treated by means of a standard matrix technique. However, in order to achieve sufficient accuracy, a second finer grid is required and therefore smaller cells having $\delta x = \frac{1}{3}$ fm and $\delta p = 40$ MeV/c are employed. The transformations between these two scales are described in Ref. [9]. We first focus on the evolution of the spatial density of the system, which is displayed in Fig. 1(a). Initially the system has a uniform density, but soon the fluctuations break this translational symmetry. Subsequently the fluctuations are rapidly amplified by the action of the effective one-body field, thus leading towards fragment formation. (Of course, real fragments do not form, because the size of the torus is kept fixed so the system cannot expand.)

It is instructive to perform a Fourier analysis of the density for the considered system, $\rho(x)$. Indeed, in the present simplified scenario, the eigenmodes of the density are plane waves, characterized by a wave number k. The amplitude associated with a given k is given by

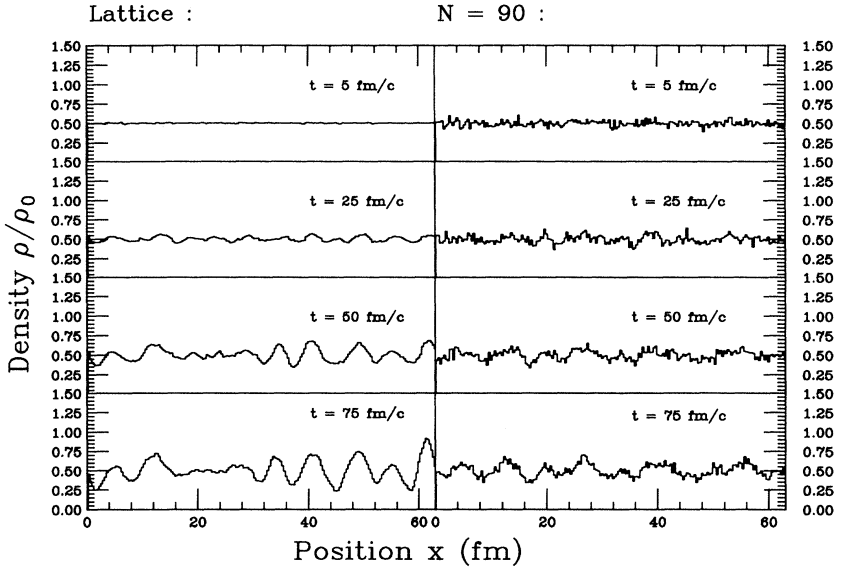

FIG. 1. Density profiles. The density profile $\rho(x,t)$ associated with one particular trajectory at four different times t, for the BL lattice calculation (a) and for the BUU test-particle simulation (b).

$$\rho(k,t) = \int_0^{L_x} dx\; e^{-ikx}\; \delta\rho(x,t)\;, \tag{7}$$

where $\delta\rho(x) = \bar{\rho}(x) - \rho_0$ represents the fluctuating part of the density and L_x is the size of the system in the x direction. The Fourier transform $\rho(k,t)$ pertains to a particular dynamical history. In reality we consider an entire ensemble of such evolutions (generated by running the code many times) and it is therefore of interest to consider the ensemble average

$$\sigma_k^2(t) = \langle |\rho(k,t)|^2 \rangle = \int\int dx\, dx'\; e^{-ik(x-x')}\; \langle \delta\rho(x,t)\; \delta\rho(x',t) \rangle\;. \tag{8}$$

This quantity is also recognized as the Fourier transform of the spatial correlation function $\sigma(x - x') = \langle \delta\rho(x,t)\; \delta\rho(x',t) \rangle$ [6].

Invoking linear response theory, we expect that the evolution of σ_k^2 is dominated by the associated unstable mode ν_k, and so it should exhibit approximately the behavior described by Eq. (4). In the present case, the eigenmodes factorize, and so $F_{\nu_k}(x,p)$ is a plane wave with respect to the position x times a function of the momentum p.

In Fig. 2(a) is shown the time evolution of σ_k^2 for the fastest growing mode. We note that while σ_k^2 is close to zero during the earliest time steps, the exponential increase predicted by Eq. (4) is clearly observed at later times. For large times $t > t_k$, we then expect that $\sigma_k^2 \approx D_k t_k \exp(2t/t_k)$ and we may then extract the key quantities D_k and t_k by simple extrapolation. This procedure gives $D_k \approx 2 \times 10^{-4}$ fm^{-3} and $t_k \approx 50$ fm/c. These values are in perfect agreement with those obtained from Eq. (3) for D_k and the dispersion relation (see Ref. [10]) for t_k.

Finally, in Fig. 3(a) we show the fluctuation σ_k^2 as a function of the wave number k. It can be seen that certain modes are amplified more rapidly than others, in accordance with their respective characteristic times t_k, and the final Fourier spectrum is therefore dominated by the most unstable modes.

B. Test-particle method

In order to test the possibility of replacing the stochastic collision term by a simple noise, we solve the BUU equation with the test-particle method, using a collisional procedure based on the concept of nucleon mean free path [11]. Since each nucleon is represented as a collection of $\mathcal{N}$ test particles, the stochasticity of the collision integral is reduced correspondingly by the factor $1/\mathcal{N}$ [8, 12]. Therefore, since $\mathcal{N}$ is always finite, the test-particle method retains some degree of fluctuation in the dynamics. Moreover, this finite sampling of the phase-space

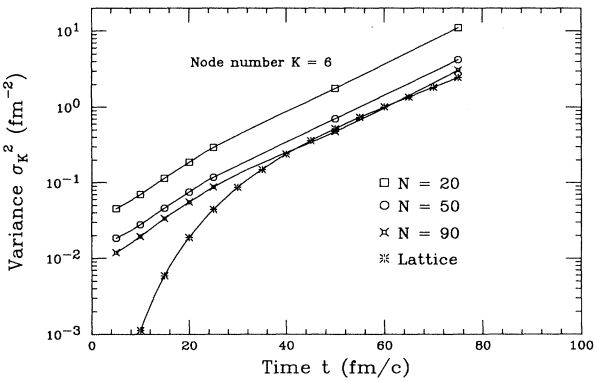

FIG. 2. Growth of the fluctuations. The time evolution of the Fourier transform of the correlation function, σ_k^2, for the most unstable mode (which has node number $K = kL_x/2\pi = 6$), for the BL lattice calculation (a) and the BUU test-particle simulation with three different values of $\mathcal{N}$, the number of test-particles per nucleon (b). This quantity is the variance of fluctuations having wave number equal to k.

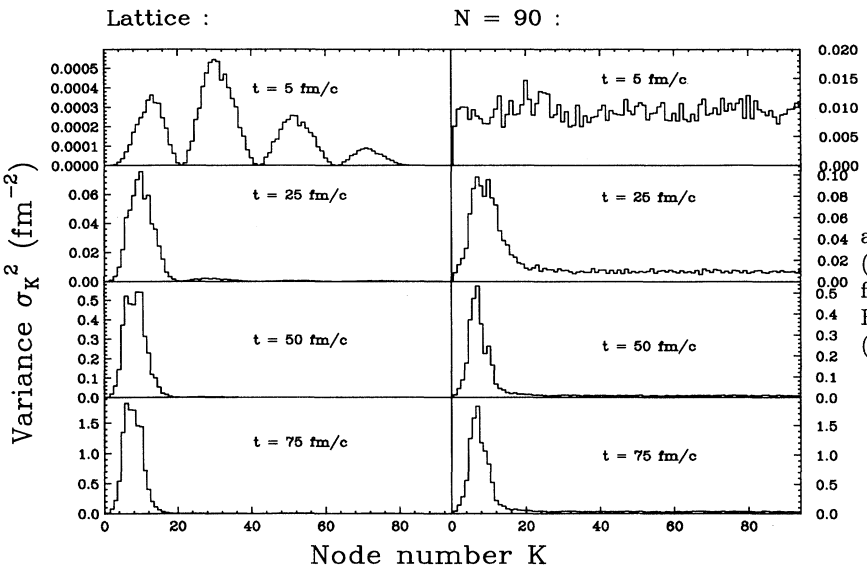

FIG. 3. Variance spectrum. The variance σ_k^2 as a function of the mode number K ($= kL_x/2\pi$), shown at a number of times t for the BL lattice calculation (a) and for the BUU test-particle simulation with $\mathcal{N} = 90$ (b).

density introduces some fluctuations in the initial conditions. When the spinodal region of the nuclear matter phase diagram is not explored, small fluctuations of the distribution function are not important because they are not amplified (but destroyed), and consequently a good description of the mean dynamics is obtained with the test-particle method [2]. By contrast, when the system is unstable, all kinds of perturbations of the density f may be important, since they are amplified, and therefore the numerics is no longer under control. This is what we observe in Fig. 1(b) where the initial noise is amplified and leads towards clusterization. In this situation our idea is to carefully adjust the numerical fluctuations (i.e., the number of test particles, $\mathcal{N}$) so as to simulate the physical fluctuations, which are well accounted in the lattice calculations (see Ref. [8] for a detailed discussion).

Since the perturbation of the density introduced by using a finite number of test particles is of statistical nature, it may be calculated in a simple manner. Thus the number of test particles, n, present in a volume V fluctuates with a characteristic dispersion $\sigma_n^2 = \bar{n}$, where $\bar{n} = \rho V \mathcal{N}$ is the mean number of test particles in V, which is fixed by the specified value of the initial density. Consequently the relative fluctuation of the density ρ is $\sigma_\rho/\rho = 1/\sqrt{\bar{n}}$ or

$$\sigma_\rho^2 = \frac{\rho^2}{\bar{n}} = \frac{n}{V^2\mathcal{N}} \,. \tag{9}$$

The corresponding Fourier coefficient (8) is then independent of k,

$$\sigma_k^2 = \frac{L_x}{L_y}\frac{\rho}{\mathcal{N}} \,. \tag{10}$$

Thus the numerical noise σ_k^2 scales as $1/\mathcal{N}$, and so it is possible to choose the number of test particles, $\mathcal{N}$, so as to reproduce the required magnitude of the physical source term D_k, for a particular value of the wave number k. Indeed, since in the BL lattice calculation we have $\sigma_k^2(0) = 0$, it follows from Eq. (4) that asymptotically (i.e., for $t \gg t_k$) the magnitude of the fluctuations is determined by $D_k t_k$, whereas it is given by $D_k t_k/\mathcal{N} + \sigma_k^2(0)$ in the BUU test-particle simulation. Therefore, the matching of those two asymptotic evolutions yields the condition

$$(\mathcal{N}-1)D_k t_k = \mathcal{N}\sigma_k^2(0) = \frac{L_x}{L_y}\rho \,, \tag{11}$$

which determines the number of test particles, $\mathcal{N}$. Inserting the values determined above for D_k and t_k, together with L_x, L_y, and ρ, we find $\mathcal{N} \approx 83$ for the fastest mode (the main uncertainty coming from the relatively inaccurate determination of the diffusion coefficient D_k).

We have then performed BUU calculations using a range of values for $\mathcal{N}$ and compared the results with the corresponding lattice calculation. The time evolution of the fastest mode is shown in Fig. 2, in addition to the corresponding BL result. The results are seen to bear out our expectation that the time evolutions follow the form given in Eq. (4). Moreover, we observe that the lattice calculation is indeed well reproduced by the BUU simulation when the value $\mathcal{N} \approx 90$ is employed, which is in excellent agreement with the above result $\mathcal{N} \approx 83$.

Figure 1(b) shows the evolution of one particular density distribution (calculated with the optimal value $\mathcal{N} = 90$), and it is seen that the density irregularities quickly attain the same magnitude as those of the lattice calculation.

In Fig. 3 we show the quantity σ_k^2 as a function of the wave number k for different times. We observe that not only are the time evolutions nearly the same, when comparing the BL lattice calculation and the BUU test-particle method, but also the spectral shapes of the fluctuations are remarkably similar. This feature is very important for the viability of the method. The similarity of the spectral shapes arises from the fact that the product $D_k t_k$ depends only relatively weakly on k, in the neighborhood of the fastest mode, so that the spectral profile depends primarily on the amplification times t_k, which are the same in the two treatments.

IV. DISCUSSION

We have shown that when one is interested in the dynamics of very unstable systems the specific character of the fluctuations may not play a decisive role in the catastrophic evolution, provided the overall magnitude of the fluctuations is suitably adjusted. This is because the various unstable modes, once they have been agitated, are amplified exponentially, so that the most unstable ones will tend to quickly dominate. In the present context, the magnitude of the imposed noise is set by the numerical parameter $\mathcal{N}$, the number of test particles per nucleon, which is determined by the relation (11). In the idealized two-dimensional case considered here, this number is around $\mathcal{N} \approx 90$. We are presently in the process of determining the value pertaining to three dimensions.

It should be noted that the source term D_k depends on the phase-space density $f(\mathbf{r}, \mathbf{p})$. For example, at relatively moderate excitations it is proportional to the square of the temperature. Consequently, the optimal value of $\mathcal{N}$, as given by Eq. (11), will depend on the process considered and should therefore be carefully adjusted for the particular scenario under study. This feature is particularly relevant in connection with the very recent calculations showing various exotic structures in central symmetric collisions [13–17], since these geometries depend sensitively on the time scale for the cluster formation, and hence the results will depend qualitatively on the particular value of $\mathcal{N}$ employed.

We wish to emphasize that in general the identification of an optimal value of $\mathcal{N}$ cannot be made as easily as in the idealized test scenario considered here. Typically, the system is undergoing a continual expansion and cooling (and it is not uniform), and the unstable modes then exhibit a more complicated dynamics. In a rough approach, one might use the method employed here to determine a range of $\mathcal{N}$ values, corresponding to the range of density and temperature the bulk of the expanding system is passing through. The corresponding set of simulations would then serve to provide bounds on the outcome of a full Boltzmann-Langevin simulation. This would already be an important advance, since no other criterion for determining a physically reasonable range of $\mathcal{N}$ values has been formulated as of yet.

Moreover, it must be noted that fluctuations are important *neither* before the system becomes unstable, since they are not amplified at this stage, *nor* after the fluctuations have grown to macroscopic size, because then their further development is dominated by the exponential amplification by the effective field. Therefore, the important physical conditions are those prevailing during a relatively brief time window of the order of t_k after the system has entered the unstable region. By studying the physical properties of the system during the collision and extracting the shortest amplification constant, it would be possible to determine that time window and to approximately match the numerical noise to the physical fluctuations over this time window, provided the physical conditions are not changing too rapidly over this period.

We wish to conclude these cautionary remarks by stressing that the method is approximate by its nature and that its utility lies more in providing a bound on the physical outcome than in making specific quantitative predictions, when the dynamical scenario is as complicated as in a typical nuclear collision.

Notwithstanding the above qualifications, the advantage of the proposed approximated test-particle method is that it makes practically possible to perform meaningful three-dimensional simulations of nuclear collisions, a task that is presently beyond feasibility for the exact Boltzmann-Langevin model.

Finally, it should be mentioned that the two-body collision integral is not the only source of fluctuations in nuclear dynamics. This fact is perhaps most evident at lower energies where the Pauli blocking renders the collision integral ineffectual, and in fact the fluctuations observed for damped reactions have been largely understood as associated with the random character of the individual nucleon transfers [18]. A suggestion is to introduce a fluctuation in the effective field, δH, which can be done already at the level of the Vlasov equation [19]. Hopefully, by confronting careful calculations based on well-controlled approximations with experimental data, it will ultimately be possible to ascertain the relative importance of the various possible mechanisms.

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